Determination of material parameters by comparison of 3D simulations and 3D experiments

Computer-based materials design plays an essential role in the development of new materials. Accurate prediction of the materials behavior during manufacturing and applications relies on accurate and complete materials databases. Traditional ways of material parameters measurements typically use idealized samples and sample environments, which may not be representative of the engineering processing and real-life usage. Moreover, material parameters are typically measured one at a time; thus it is time-consuming and costly to measure material parameters with large spectrum.

In this thesis, a fitting methodology is proposed to determine material parameters by comparison between 4D x-ray experiments and phase-field simulations. The evolution of material microstructures is measured at a condition that mimics realistic engineering manufacturing and applications with 3D non-destructive in situ x-ray techniques. Starting from one snapshot of the experimental microstructure, the evolution of the 3D material microstructure is simulated using a phase-field model. An iterative optimization technique is used to find the values of material parameters that yield the best match between the simulated microstructure and the measured microstructure in a global manner. The proposed method is demonstrated on a simple case to fit two material parameters: the liquid diffusion coefficient and the capillary length of a hypoeutectic Al-Cu alloy, and a complicated case to fit hundreds of material parameters: the reduced grain boundary mobilities of pure iron. Results show that the proposed method is capable of providing reliable measurements of material parameters that are difficult to measure in traditional ways and can determine many - possibly all relevant - values of material parameters simultaneously. Moreover, the method developed is broadly applicable to many materials systems and experiments that provide 3D microstructure evolution.

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